1,3-dibromoadamantane

Inchi: InChI=1S/C10H14Br2/c11-9-2-7-1-8(4-9)5-10(12,3-7)6-9/h7-8H,1-6H2
InchiKey: HLWZKLMEOVIWRK-UHFFFAOYSA-N
Formula: C10H14Br2
SMILES: BrC12CC3CC(C1)CC(Br)(C3)C2
Mol. weight [g/mol]: 294.03
CAS: 876-53-9

Physical Properties

Property code	Value	Unit	Source
gf	213.42	kJ/mol	Joback Method
hf	25.31	kJ/mol	Joback Method
hfus	13.01	kJ/mol	Joback Method
hvap	48.02	kJ/mol	Joback Method
log10ws	-4.30		Crippen Method
logp	3.868		Crippen Method
mcvol	154.180	ml/mol	McGowan Method
pc	4067.32	kPa	Joback Method
rinpol	1590.00		NIST Webbook
rinpol	1590.00		NIST Webbook
ripol	2264.00		NIST Webbook
ripol	2264.00		NIST Webbook
ripol	2264.00		NIST Webbook
tb	580.82	K	Joback Method
tc	847.96	K	Joback Method
tf	415.92	K	Joback Method
vc	0.578	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	366.43	J/mol×K	580.82	Joback Method
cpg	383.20	J/mol×K	625.34	Joback Method
cpg	398.43	J/mol×K	669.87	Joback Method
cpg	412.65	J/mol×K	714.39	Joback Method

cpg	426.40	J/mol×K	758.91	Joback Method
cpg	440.21	J/mol×K	803.43	Joback Method
cpg	454.63	J/mol×K	847.96	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C876539&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume